Letters to the Editor

Indian J. Phys. **51A**, 303–304 (1977)

Crystallographic studies of ortho-cyanobenzyl bromide

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(*Received* 18 *November* 1976, *revised* 20 *January* 1977)

The compound of ortho cynobenzyl bromide was first prepared by Drory (Drory 1891) and later by Reynold C. Fuson (Fuson 1926) by applying different methods. The chemical formula of the compound is

C_8H_6 B N. and the melting point 71·5°C–72·5°C

Under ordinary light the crystals were colourless and transparent and of rectangular shape. Under crossed nicols it gave interference colour and showed oblique extinction, the angle of extinction being 28°30′. The crystal was also observed to be length fast and change in relief was noted when the polariser was rotated. Since no X-ray investigation of this crystal has been made as yet, an attempt has been made to carry out full X-ray investigations to solve its structure.

Since the crystal was found to decompose when exposed to ordinary atmospheric conditions it was sealed in a Lindemann Glass Capillaries of 0·5 mm bore for the purpose of taking rotation and Weissenberg photographs

The unit cell dimensions (Henry, Lipson & Wooster 1951) as determined from rotation and Weissenberg photographs are, $a = 7{\cdot}248$Å, $b = 8{\cdot}160$Å, $c = 12{\cdot}690$Å, $\beta = 98{\cdot}2°$.

From the indexed Weissenberg photographs (Jeffery 1971) the following systematic absences of reflections were observed :

hkl : no condition
hol : $l = 2n+1$
oko : $k = 2n+1$

and hence the space group $P2_1/C$ was assigned to the crystal. The density of the crystal as determined by the method of floatation with $ZnCl_2$ solution was 1·708 gm/cc. and calculated density assuming four formula units per unit cell of C_8H_6B N was 1·718 gm/cc.

Intensity data along a-axis and zero layer photograph about b-baxis were collected using non-integrated equi-inclination Weissenberg photographs using Copper radiation. The intensity of the spots were measured by eye-estimations against a prepared standard intensity scale. Symmetry related reflections were averaged to reduce the error caused by spot extension and contraction. The intensities for different layers were also corrected for spot size and Lorentz polarisation factors.

Patterson projection on (100) shown in figure (1) has been computed with the help of Robertson strips and the positions of the bromine atoms in the unit cell were located (Buerger 1960) and this was then used to phzase the observed structure factors of all *okl* reflections and Fourier projection on (100) was calculated where bromine atoms and some of the other atoms have appeared. Further investigations are in progress and will appear shortly.

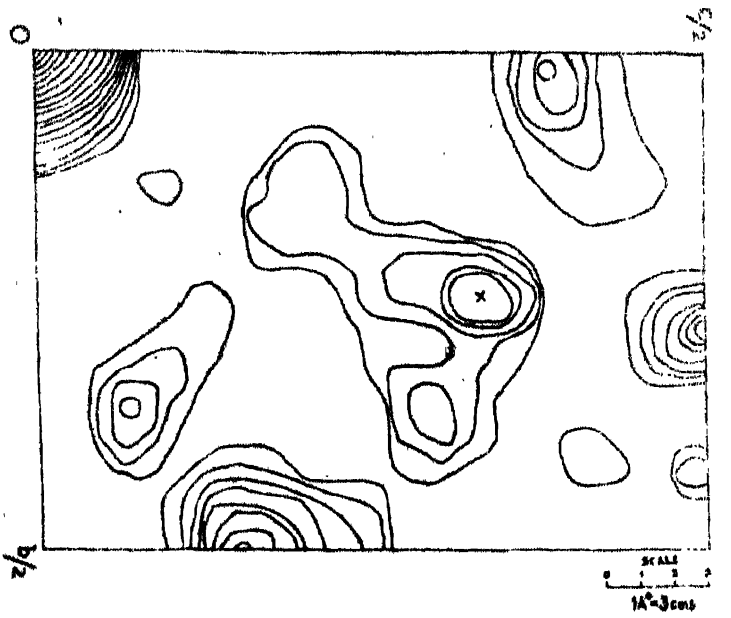

Fig 1 Patterson synthesis of ortho-cyanobenzyl bromide projected on (100) The BR-BR-peak is indicated by crosses

One of the authors A. C. Dutta is grateful to the government of Bihar, Department of Science and Technology, for the grant of salaried leave with scholarship.

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